

Quantification of Uncertainties in Nuclear Density Functional theory

N. Schunck,^{1,*} J.D. McDonnell,¹ D. Higdon,² J. Sarich,³ and S. Wild³

¹*Physics Division, Lawrence Livermore National Laboratory, Livermore, CA, 94551, USA*

²*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

³*Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, USA*

(Dated: September 19, 2014; Received XX May 2014; revised received XX August 2014; accepted XX September 2014)

Reliable predictions of nuclear properties are needed as much to answer fundamental science questions as in applications such as reactor physics or data evaluation. Nuclear density functional theory is currently the only microscopic, global approach to nuclear structure that is applicable throughout the nuclear chart. In the past few years, a lot of effort has been devoted to setting up a general methodology to assess theoretical uncertainties in nuclear DFT calculations. In this paper, we summarize some of the recent progress in this direction. Most of the new material discussed here will be published in separate articles.

I. INTRODUCTION

The rapid development of leadership class computing facilities throughout the world, accompanied by targeted programs from funding agencies to foster the use of high-performance computing methods in science, have opened new opportunities in theoretical nuclear structure [1]. It has become possible to address important questions of nuclear science using microscopic approaches to structure and reaction rooted in the knowledge of effective nuclear forces and standard methods of quantum mechanics. Recent examples include the explanation of the anomalously long half-life of ^{14}C isotope used in carbon-dating [2], predictions of neutrino-nucleus currents relevant to physics beyond the standard model [3], or of light ion fusion reactions relevant to the National Ignition Facility [4], to name but a few.

In parallel, there has been an increasing need for accurate and precise data, whether from measurements or simulations, in areas as diverse as nuclear astrophysics [5, 6], reactor physics [7] or data evaluation [8]. In the past, the cost of using standard methods of statistics to estimate theoretical uncertainties in such microscopic approaches was often prohibitive, but this limitation has slowly been disappearing.

Among the few microscopic theories of nuclear structure, density functional theory (DFT) plays a special role, since it is the only one to be applicable across the entire nuclear chart, from the lightest to the heaviest elements. Therefore, DFT is the tool of choice to study phenomena such as nuclear fission [9] or superheavy element predictions [10], but has also seen applications in tests of funda-

mental symmetries [11, 12] or the search for neutrino-less double beta-decay [13].

In this proceeding, we briefly present some of the challenges and methodologies used in nuclear DFT to estimate theoretical uncertainties. This topic is covered in greater details in an invited contribution to a Focus Issue of the Journal of Physics G: Nuclear and Particle Physics on “Enhancing the Interaction Between Nuclear Experiment and Theory Through Information and Statistics” [14–16]. In section II, we recall the main components of nuclear DFT. In section III, we summarize some of the recent results in uncertainty quantification and error propagation, before we conclude in section IV.

II. NUCLEAR DENSITY FUNCTIONAL THEORY

Density functional theory (DFT) is a general approach to the quantum many-body system. It is based on a series of theorems by Kohn and Sham, who have shown that it is theoretically possible to find the exact ground-state energy of a system of N interacting electrons by solving a system of equations characteristic of an independent particle system [17, 18]. This existence theorem was later extended to the context of nuclear physics [19]. Nuclear DFT is a reformulation of the traditional self-consistent mean-field (SCMF) theory of nuclear structure, which has been very successful in predicting a broad range of nuclear properties.

The essential component of both the SCMF theory and nuclear DFT is the energy density functional (EDF), which encapsulates all information about the system (in principle). The EDF is a functional of the density of neutrons and protons, as well as of the pairing density [20].

* Corresponding author: schunck1@llnl.gov

In nuclear DFT, the EDF is treated at the Hartree-Fock-Bogoliubov (HFB) approximation [21]; in the SCMF, the EDF is often related to an underlying two-body Hamiltonian, and the HFB approximation may be only the first step of a series of calculations [22]. In any case, the EDF is characterized by a number of coupling constants which are not given by any underlying theory and must therefore be adjusted to some experimental data.

One must emphasize that the Kohn-Sham theorem is only an existence theorem: there is no magic recipe to determine the one EDF that will give the exact energy of the nucleus. In addition, in-medium nuclear forces are poorly known and should in principle be derived from quantum chromodynamics. This is in contrast to electronic DFT, where the Coulomb force is known exactly. For these reasons, one should, therefore, consider nuclear DFT (and the SCMF) as inherently imperfect models of the nucleus: this is the first, major source of errors in DFT, which we will refer to as “model errors”. Let us denote by $\mathbf{x} = (x_1, \dots, x_{n_x})$ the parameters of the EDF, aka the model. Typically, $n_x \approx 10 - 20$. These parameters will be fitted on some n_d data points y_i . There could be different types of data: atomic masses, r.m.s. charge radii, mass differences, excitation energies of isomers, etc. It is clear that, given a specific EDF, the choice of the experimental data will impact the overall predictive power of DFT: this is the second source of errors in DFT, which we will label “fitting errors”. Finally, there is a third source of errors, “implementation errors”, caused by the need to solve the DFT equations numerically. These various sources of uncertainties are discussed in more details in [14]. In this proceeding, we focus only on selected aspects of fitting errors.

III. QUANTIFYING AND PROPAGATING ERRORS IN NUCLEAR DFT

As already mentioned above, we will only discuss uncertainties pertaining to the determination of model parameters. We thus assume we have an energy density functional, which is characterized by the n_x unknown parameters \mathbf{x} . We are trying to determine the best way to obtain an optimal set of parameters \mathbf{x} and, in the same time, to quantify the uncertainties associated with this procedure.

We recall that there is a very large amount of experimental data that potentially could be used to fit the few parameters of an EDF. However, different data types may have very different impacts on specific model parameters. For example, it was pointed out using a singular value decomposition analysis that only a few of the eight parameters of a standard Skyrme EDF are really relevant to reproduce nuclear masses [23] or single-particle energies [24]. In order to constrain every coupling constant of the EDF, it thus appears necessary to introduce different types of data. In practice, the determination of EDF parameters is thus made by minimizing the composite χ^2

function

$$\chi^2(\mathbf{x}) = \frac{1}{n_d - n_x} \sum_{t=1}^{n_T} \sum_{j=1}^{n_t} \left(\frac{y_{tj}(\mathbf{x}) - d_{tj}}{\sigma_t} \right)^2, \quad (1)$$

with n_T the number of different data types, n_t the number of data points for type t , and $n_d = \sum_t n_t$ the total number of data points over all types. The calculated value of data point number j of type t is denoted by y_{tj} , with d_{tj} the corresponding experimental value. Because there are different types of data, relative distances must be properly normalized by the quantity σ_t , which represents an estimate of the theoretical error on data type t . This strategy was followed in a series of paper by the UNEDF collaboration [25–27].

The minimization of the χ^2 function gives access to the “optimal” parametrization of the EDF. Obviously, one should bear in mind that this optimal choice is strongly dependent on (i) the choice of the types t of experimental data, (ii) the number of data points for each type t , (iii) the weight σ_t chosen for each type. In addition, the quality of the optimization is contingent of the algorithm used and depends on the starting point. Bearing in mind these caveats, it is possible to estimate the covariance matrix by assuming normally distributed errors and approximate linear variations of the χ^2 function under variations of model parameters [28]. This approximation has often been used to propagate model errors [29–32].

Very recently, alternative approaches to uncertainty quantification based on Bayesian statistics have been investigated for semi-microscopic nuclear mass models based [33]. In the context of nuclear DFT, such approaches are appealing since they treat model parameters as intrinsically random variables, the true value of which can not be known with certainty. This perspective is particularly adapted to nuclear structure theory, since the nuclear many-problem is unsolvable exactly: only approximations are available (DFT is one of them), and, therefore, uncertainties are unavoidable and should be quantified. Mathematical details on how posterior distributions can be generated in the context of nuclear DFT are discussed in details in [16]; a paper currently being finalized by our group also uses Bayesian posteriors to analyze theoretical uncertainties for the prediction of neutron-drip lines and fission barriers in actinides [34].

We show in Fig. 1 one of the first examples of a Bayesian posterior distribution corresponding to the UNEDF1 χ^2 function of [27]. The red dots correspond to the UNEDF1 solution itself. Obtaining such distributions requires first to set up intervals of variations $[x_i^{\min}, x_i^{\max}]$ for each of the DFT parameters. These intervals define a 12-d hypercube in parameter space from which the prior distribution is sampled. In the case shown in Fig. 1, the interval for each parameter x_i was defined as $[x_i^* - 3\sigma_i, x_i^* + 3\sigma_i]$, with x_i^* the UNEDF1 value and σ_i its standard deviation; see [26]. Since this work is still exploratory, we chose a uniform prior distribution. Because of the significant cost of running the DFT calculation of the UNEDF1 χ^2 (about 800 cores for 15 minutes),

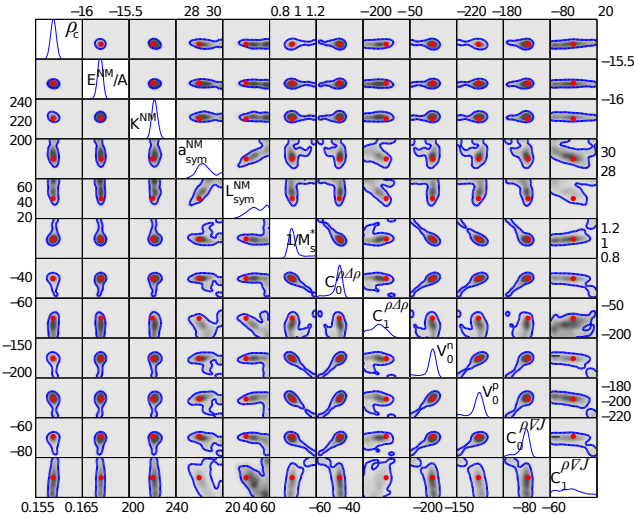


FIG. 1. (Color online) Univariate and bivariate marginal estimates of the posterior distribution for the 12-dimensional DFT parameter vector \mathbf{x} of the UNEDF1 parametrization. The blue line encloses an estimated 95% region. .

the posterior was extracted from a response function constructed using Gaussian Process techniques; see [16] for a full description of the method. The response function was based on 200 DFT calculations of the χ_2 sampling the 12-d hypercube.

Once the posterior distribution for the DFT model parameters is known, we can estimate theoretical error bars of an observable \mathcal{O} by computing it for a sample $\mathcal{S} = (\mathbf{x}_1, \dots, \mathbf{x}_s)$ of DFT parameter sets drawn from the posterior. As mentioned earlier, we will present the results of such a strategy for neutron drip lines and fission barriers elsewhere [34]. In this proceeding, we illustrate the approach with the preliminary example of the proton r.m.s. radii in 27 spherical nuclei used in the fit of the UNEDF family of functionals. Fig. 2 shows the estimate of theoretical errors obtained from the Bayesian analysis relative to the UNEDF1 values. Black marks are the experimental values of the radius. The dark blue band shows the 90% prediction uncertainty (including emulator error). The light blue band also includes the fitting error, i.e., the discrepancy between the actual experimental data and the DFT calculation – assumed to follow a normal distribution. The outlier at $Z=50, N=64$ hints at systematic errors, i.e. the inability of the model to reproduce the data, irrespective of how model parameters are fitted.

IV. CONCLUSIONS

In many important research areas and contemporary applications of nuclear science, nuclear density functional theory represents the only microscopic model of structure and reactions available. In this proceeding, we have briefly summarized some of the challenges and recent re-

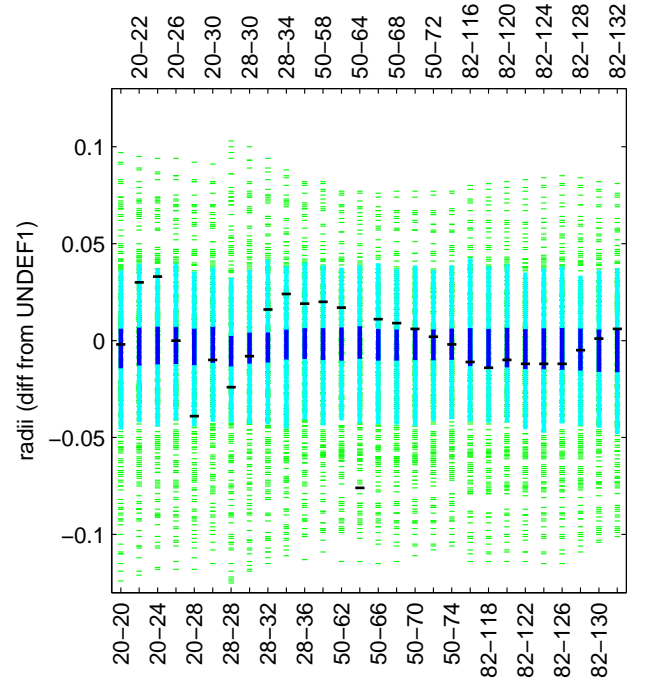


FIG. 2. (Color online) Estimates of theoretical uncertainties for proton radii in 27 spherical Ca, Ni, Sn and Pb isotopes relative to the UNEDF1 parametrization of the Skyrme functional. Nuclei are labeled $Z-N$. Black marks are experimental values, the dark blue band the 90% prediction interval of the model alone, the light blue band the 90% prediction interval when also including fitting errors of the model.

sults in identifying and quantifying theoretical uncertainties inherent to nuclear DFT. In particular, we have emphasized the widespread use of covariance analysis and the first applications of Bayesian statistics in DFT. With the constant development of supercomputers, such methods will most likely gain in popularity and could be applied, e.g., to practical applications such as the quantification of errors for fission product yields in neutron-induced fission.

Acknowledgements: This work was partly performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. It was supported by the SciDAC activity within the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research program under contract number DE-AC02-06CH11357. Computational resources were provided through an INCITE award “Computational Nuclear Structure” by the National Center for Computational Sciences (NCCS) and National Institute for Computational Sciences (NICS) at Oak Ridge National Laboratory, through an award by the Livermore Computing Resource Center at Lawrence Livermore National Laboratory, and through an award by the Laboratory Computing Resource Center at Argonne National Laboratory.

- [1] S. Bogner, A. Bulgac, J. Carlson, J. Engel, G. Fann, R. J. Furnstahl, S. Gandolfi, G. Hagen, M. Horoi, and C. Johnson, “Computational nuclear quantum many-body problem: The UNEDF project,” *COMPUT. PHYS. COMM.* **84**, 2235 (2013).
- [2] P. Maris, J. P. Vary, P. Navrátil, W. E. Ormand, H. Nam, and D. J. Dean, “Origin of the Anomalous Long Lifetime of ^{14}C ,” *PHYS. REV. LETT.* **106**, 202502 (2011).
- [3] A. Lovato, S. Gandolfi, J. Carlson, S. C. Pieper, and R. Schiavilla, “Neutral Weak Current Two-Body Contributions in Inclusive Scattering from ^{12}C ,” *PHYS. REV. LETT.* **112**, 182502 (2014).
- [4] P. Navrátil, and S. Quaglioni, “Ab Initio Many-Body Calculations of the $^3\text{H}(d, n)^4\text{He}$ and $^3\text{He}(d, p)^4\text{He}$ Fusion Reactions,” *PHYS. REV. LETT.* **108**, 042503 (2012).
- [5] F. Käppeler, R. Gallino, S. Bisterzo, and W. Aoki, “The s process: Nuclear physics, stellar models, and observations,” *REV. MOD. PHYS.* **83**, 157 (2011).
- [6] K. Langanke and G. Martínez-Pinedo, “Nuclear weak-interaction processes in stars,” *REV. MOD. PHYS.* **75**, 819 (2003).
- [7] C. Ceresio, O. Cabellos, J. S. Martínez, and C. J. Diez, “Importance of Nuclear Data Uncertainties in Criticality Calculations,” *EPJ WEB OF CONFERENCES* **27**, 00004 (2012).
- [8] M. Herman and A. Koning, “Covariance data in the fast neutron region,” Tech. Rep. 24, Technical report NEA/WPEC-24, OECD Nuclear Energy Agency, Paris (2011).
- [9] W. Younes and D. Gogny, “Nuclear scission and quantum localization,” *PHYS. REV. LETT.* **107**, 132501 (2011).
- [10] S. Hofmann and G. Münzenberg, “The discovery of the heaviest elements,” *REV. MOD. PHYS.* **72**, 733 (2000).
- [11] J. Dobaczewski and P. Olbratowski, “Nuclear Time-Reversal Violation and the Schiff Moment of $\text{Ra}225$,” *PHYS. REV. LETT.* **94**, 23 (2005).
- [12] S. Ban, J. Dobaczewski, J. Engel, and A. Shukla, “Fully self-consistent calculations of nuclear schiff moments,” *PHYS. REV. C* **82**, 015501 (2010).
- [13] T. R. Rodríguez and G. Martínez-Pinedo, “Energy density functional study of nuclear matrix elements for neutrinoless $\beta\beta$ decay,” *PHYS. REV. LETT.* **105**, 252503 (2010).
- [14] Nicolas Schunck, Jordan D McDonnell, Jason Sarich, Stefan M Wild, Dave Higdon, “Error analysis in nuclear density functional theory,” arXiv:1407.3017, *J. PHYS. G: NUCL. PART. PHYS.* (2014). To be published.
- [15] Stefan M Wild, Jason Sarich, Nicolas Schunck, “Derivative-free optimization for parameter estimation in computational nuclear physics,” arXiv:1406.5464, *J. PHYS. G: NUCL. PART. PHYS.* (2014). To be published.
- [16] Dave Higdon, Jordan D McDonnell, Nicolas Schunck, Jason Sarich, Stefan M Wild, “A Bayesian Approach for Parameter Estimation and Prediction using a Computationally Intensive Model,” arXiv:1407.3017, *J. PHYS. G: NUCL. PART. PHYS.* (2014). To be published.
- [17] P. Hohenberg and W. Kohn, “Inhomogeneous electron gas,” *PHYS. REV.* **136**, B864 (1964).
- [18] W. Kohn and L. J. Sham, “Self-Consistent equations including exchange and correlation effects,” *PHYS. REV.* **140**, A1133 (1965).
- [19] J. Messud, M. Bender, and E. Suraud, “Density functional theory and Kohn-Sham scheme for self-bound systems,” *PHYS. REV. C* **80**, 054314 (2009).
- [20] E. Perlińska, S. Rohoziński, J. Dobaczewski, and W. Nazarewicz, “Local density approximation for proton-neutron pairing correlations: Formalism,” *PHYS. REV. C* **69**, 014316 (2004).
- [21] P. Ring and P. Schuck, *THE NUCLEAR MANY-BODY PROBLEM*. Springer-Verlag, (2000).
- [22] M. Bender, P. Heenen, and P. Reinhard, “Self-consistent mean-field models for nuclear structure,” *REV. MOD. PHYS.* **75**, 121 (2003).
- [23] G. Bertsch, B. Sabbey, and M. Uusnäkki, “Fitting theories of nuclear binding energies,” *PHYS. REV. C* **71**, 054311 (2005).
- [24] M. Kortelainen, J. Dobaczewski, K. Mizuyama, and J. Toivanen, “Dependence of single-particle energies on coupling constants of the nuclear energy density functional,” *PHYS. REV. C* **77**, 064307 (2008).
- [25] M. Kortelainen, J. McDonnell, W. Nazarewicz, E. Olsen, P. Reinhard, J. Sarich, N. Schunck, S. M. Wild, D. Davesne, J. Erler, and A. Pastore, “Nuclear energy density optimization: Shell structure,” *PHYS. REV. C* **89**, 054314 (2014).
- [26] M. Kortelainen, J. McDonnell, W. Nazarewicz, P. Reinhard, J. Sarich, N. Schunck, M. V. Stoitsov, and S. M. Wild, “Nuclear energy density optimization: Large deformations,” *PHYS. REV. C* **85**, 024304 (2012).
- [27] M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, and S. Wild, “Nuclear energy density optimization,” *PHYS. REV. C* **82**, 024313 (2010).
- [28] J. Dobaczewski, W. Nazarewicz, and P. Reinhard, “Error estimates of theoretical models: a guide,” *J. PHYS. G: NUCL. PART. PHYS.* **41**, 074001 (2014).
- [29] P. Reinhard, J. Piekarewicz, W. Nazarewicz, B. K. Agrawal, N. Paar, and X. Roca-Maza, “Information content of the weak-charge form factor,” *PHYS. REV. C* **88**, 034325 (2013).
- [30] J. Piekarewicz, B. K. Agrawal, G. Colò, W. Nazarewicz, N. Paar, P. Reinhard, X. Roca-Maza, and D. Vretenar, “Electric dipole polarizability and the neutron skin,” *PHYS. REV. C* **85**, 041302 (2012).
- [31] P. Reinhard and W. Nazarewicz, “Information content of the low-energy electric dipole strength: Correlation analysis,” *PHYS. REV. C* **87**, 014324 (2013).
- [32] M. Kortelainen, J. Erler, W. Nazarewicz, N. Birge, Y. Gao, and E. Olsen, “Neutron-skin uncertainties of skyrme energy density functionals,” *PHYS. REV. C* **88**, 031305 (2013).
- [33] S. Goriely and R. Capote, “Uncertainties of mass extrapolations in Hartree-Fock-Bogoliubov mass models,” *PHYS. REV. C* **89**, 054318 (2014).
- [34] J. McDonnell, N. Schunck, D. Higdon, W. Nazarewicz, J. Sarich, and S. Wild, “Error analysis in nuclear density functional theory.” In preparation (2014).